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Subject: SAB2002 - An S(a,b) Library for MCNP

Introduction

A new $S(\alpha,\beta)$ neutron thermal library has been created for MCNP [1]. The library, named SAB2002, contains thermal scattering data for 15 moderators based on the latest ENDF/B-VI evaluations [2]. The data are available at a variety of temperatures.

Evaluated Data

ENDF/B-VI Release 3 includes neutron thermal scattering data for 15 moderators: beryllium metal, beryllium oxide, graphite, polyethylene, benzene, light water, heavy water, hydrogen and zirconium in zirconium hydride, ortho and para hydrogen, ortho and para deuterium, and liquid and solid methane. Evaluated data for three of the materials (polyethylene, benzene, and heavy water) were carried over from previous versions of ENDF/B [3]. Evaluated data for the remaining 12 moderators were updated for ENDF/B-VI Release 3 [4].

NJOY Processing

The NJOY processing code system [5] was used to create $S(\alpha,\beta)$ tables for MCNP from the ENDF/B evaluations. NJOY versions 99.0, 99.10, and 99.50 were used (in particular, Version 99.50 was used for the four tables processed in 2003 – results were equivalent to those from earlier versions). The primary NJOY modules involved in this job are THERMR and ACER. The maximum neutron energy is 4.5 eV for Be, BeO, graphite, poly, H_2O , D_2O , H and Zr in ZrH, and benzene. The maximum neutron energy is 1.0 eV for liquid and solid methane. The maximum neutron energy is 0.5 eV for para and ortho H and for para and ortho H.

MCNP Data Tables

A total of 64 MCNP data tables has been created for the 15 moderators. Information about these 64 tables similar to that contained in Appendix G of the MCNP manual is provided here in Table 1. Note that these data tables may be used with any modern version of MCNP; however Version 5 of MCNP is required to correctly utilize the "zr/h" tables when the user specifies multiple isotopes of Zr (as opposed to elemental Zr) on the MCNP Mn card.

Table 1 – MCNP Data Tables on the SAB2002 Library

Benzene (1001,	6000, 6012)						
benz.60t	endf6.3	sab2002	09/14/99	294.	16	64	none
benz.61t	endf6.3	sab2002	09/14/99	400.	16	64	none
benz.62t	endf6.3	sab2002	09/14/99	600.	16	64	none
benz.63t	endf6.3	sab2002	09/14/99	800.	16	64	none
Beryllium Oxid	e (4009, 8016	5)					

beo.60t	endf6.3	sab2002	09/14/99	294.	16	64	coh
beo.61t	endf6.3	sab2002	09/14/99	400.	16	64	coh
beo.62t	endf6.3	sab2002	09/14/99	600.	16	64	coh
beo.63t	endf6.3	sab2002	09/14/99	800.	16	64	coh
beo.64t	endf6.3	sab2002	09/14/99	1000.	16	64	coh
beo.65t	endf6.3	sab2002	09/14/99	1200.	16	64	coh
200.030	CHGI 0.3	Babboob	03/11/33	1200.			0011
Beryllium Meta	1 (4009)						
be.60t	endf6.3	sab2002	09/13/99	294.	16	64	coh
be.61t	endf6.3	sab2002	09/13/99	400.	16	64	coh
be.62t	endf6.3	sab2002	09/13/99	600.	16	64	coh
be.63t	endf6.3	sab2002	09/14/99	800.	16	64	coh
be.64t	endf6.3	sab2002	09/14/99	1000.	16	64	coh
be.65t	endf6.3	sab2002	09/14/99	1200.	16	64	coh
be.69t	endf6.3	sab2002	09/17/99	77.	16	64	coh
Deuterium in He	eavy Water (1002)					
hwtr.60t	endf6.3	sab2002	09/14/99	294.	16	64	none
hwtr.61t	endf6.3	sab2002	01/20/03	400.	16	64	none
hwtr.62t	endf6.3	sab2002	09/14/99	600.	16	64	none
hwtr.63t	endf6.3	sab2002	09/14/99	800.	16	64	none
hwtr.64t	endf6.3	sab2002	01/20/03	1000.	16	64	none
Graphite (6000	, 6012)						
grph.60t	endf6.3	sab2002	09/14/99	294.	16	64	coh
grph.61t	endf6.3	sab2002	09/14/99	400.	16	64	coh
grph.62t	endf6.3	sab2002	09/14/99	600.	16	64	coh
grph.63t	endf6.3	sab2002	09/14/99	800.	16	64	coh
grph.64t	endf6.3	sab2002	09/14/99	1000.	16	64	coh
grph.65t	endf6.3	sab2002	09/14/99	1200.	16	64	coh
Hydrogen in Lig	ght Water (10	001)					
lwtr.60t	endf6.3	sab2002	09/13/99	294.	16	64	none
lwtr.61t	endf6.3	sab2002	09/13/99	400.	16	64	none
lwtr.62t	endf6.3	sab2002	09/13/99	600.	16	64	none
lwtr.63t	endf6.3	sab2002	09/13/99	800.	16	64	none
lwtr.64t	endf6.3	sab2002	01/21/03	1000.	16	64	none
Hydrogen in Po	lyethylene (1						
poly.60t	endf6.3	sab2002	09/14/99	294.	16	64	inco
Hydrogen in Zi:			00/14/22				
h/zr.60t	endf6.3	sab2002	09/14/99	294.	16	64	inco
h/zr.61t	endf6.3	sab2002	09/14/99	400.	16	64	inco
h/zr.62t	endf6.3	sab2002	09/14/99	600.	16	64	inco
h/zr.63t	endf6.3	sab2002	09/14/99	800.	16	64	inco
h/zr.64t	endf6.3	sab2002	09/14/99	1000.	16	64	inco
h/zr.65t	endf6.3	sab2002	09/14/99	1200.	16	64	inco
		(1007)					
Hydrogen in Lie		(1001)	00/1=/00	100			
lmeth.60t	endf6.3	sab2002	09/17/99	100.	16	64	none
Ontho Doutsel	m (1002)						
Ortho Deuterium		anh0000	00/16/00	1.0	1 (<i>C</i> A	n.c
dortho.60t	endf6.3	sab2002	09/16/99	19.	16	64	none
Ortho Hydrogen	(1001)						
hortho.60t	endf6.3	sab2002	01/21/03	1.0	1 <i>C</i>	6.1	nono
1101 (110.00)	enaro.s	SabZUUZ	01/21/03	19.	16	64	none

hortho.61t hortho.62t	endf6.3						
hortho.62t	G1101.0.2	sab2002	06/14/00	20.	16	64	none
1101 0110 1 010	endf6.3	sab2002	06/14/00	21.	16	64	none
hortho.63t	endf6.3	sab2002	06/14/00	22.	16	64	none
hortho.64t	endf6.3	sab2002	06/14/00	23.	16	64	none
hortho.65t	endf6.3	sab2002	06/14/00	24.	16	64	none
hortho.66t	endf6.3	sab2002	06/14/00	25.	16	64	none
Para Deuterium	(1002)						
dpara.60t	endf6.3	sab2002	09/16/99	19.	16	64	none
Para Hydrogen	(1001)						
hpara.60t	endf6.3	sab2002	06/14/00	19.	16	64	none
hpara.61t	endf6.3	sab2002	06/13/00	20.	16	64	none
hpara.62t	endf6.3	sab2002	06/14/00	21.	16	64	none
hpara.63t	endf6.3	sab2002	06/14/00	22.	16	64	none
hpara.64t	endf6.3	sab2002	06/14/00	23.	16	64	none
hpara.65t	endf6.3	sab2002	06/14/00	24.	16	64	none
hpara.66t	endf6.3	sab2002	06/14/00	25.	16	64	none
Hydrogen in So	lid Methane (1001)					
smeth.60t	endf6.3	sab2002	09/17/99	22.	16	64	inco
Zirconium in Z	irconium Hydr	ride (40000,	40090, 40091,	40092,	40094,	40096)	
zr/h.60t	endf6.3	sab2002	09/14/99	294.	16	64	inco
	endf6.3	sab2002	09/14/99	400.	16	64	inco
zr/h.61t	21141 0 . 3						
zr/h.61t zr/h.62t	endf6.3	sab2002	09/14/99	600.	16	64	inco
•		sab2002 sab2002	09/14/99 09/14/99	600. 800.		64	inco
zr/h.62t	endf6.3				16		

Given in parenthesis are the nuclides for which the $S(\alpha,\beta)$ data are valid. For example, lwtr.60t provides scattering data only for 1H ; ^{16}O would still be represented by the default free-gas treatment.

The first column of Table 1 contains the ZAID, which is the table identification to be specified on MCNP MTn cards. The portion of the ZAID before the decimal point provides a shorthand alphanumeric description of the material. The two digits after the decimal point differentiate among different tables for the same material. The final character in the ZAID is a "t" which indicates thermal $S(\alpha,\beta)$ table.

The second column of Table 1 is the evaluated source. For the SAB2002 library, all data are from ENDF/B-VI Release 3.

The third column is the library name; here, obviously, always SAB2002.

The fourth column provides the date that the data table was processed by the NJOY code.

The fifth column is the temperature of the data (in degrees Kelvin).

The sixth column contains the number of equally-likely discrete secondary cosines provided at each combination of incident and secondary energy for inelastic scattering, and for each incident energy for incoherent elastic scattering. Note that this value (16) is substantially larger than that for previous MCNP thermal data tables, leading to more resolution in the data.

The seventh column gives the number of secondary energies provided for each incident energy for inelastic scattering. Note that this value (64) is substantially larger than that for previous MCNP thermal data tables, leading to more resolution in the data.

There are three options for the elastic scattering entry in the eighth column:

none -- no elastic scattering data for this material.

coh -- coherent elastic scattering data provided for this material (Bragg scattering).

inco - incoherent elastic scattering data provided for this material.

Verification and Validation

Only very minor changes to the tables generated by NJOY were required, generally involving updates to the list of integer nuclides for which the $S(\alpha,\beta)$ data are valid. Cross sections for each moderator have been plotted for each temperature and each reaction. Average scattering energies and angles have been constructed and plotted. All data tables have been run in standard MCNP problems. Several data tables have been used to calculate various criticality benchmarks [6]. No problems have been identified.

Comparison to Previous MCNP Thermal Libraries

There are two previous MCNP thermal $S(\alpha,\beta)$ libraries. The TMCCS library contains data for 9 moderators (Be, BeO, H_2O , D_2O , benzene, poly, graphite, and H and Zr in ZrH) based on ENDF/B-V. Note that these evaluations had been carried over from ENDF/B-III [3]. The THERXS library contains data for 6 cold moderators based on initial work performed ~ 1989 at Los Alamos [7,8].

The cross sections for the bulk of the reactor moderator materials show only modest differences on SAB2002 compared with TMCCS. There is an improvement in the inelastic scattering cross section for H in ZrH. On the other hand, almost all of the cold moderators (with the exception of liquid methane) show substantial improvements from the data on THERXS. Finally, all data tables on SAB2002 include more detailed resolution than previous libraries in terms of secondary neutron energies and scattering angles.

Summary

A new MCNP thermal $S(\alpha,\beta)$ library has been created, verified, and made available to users. The library is named SAB2002 and contains a total of 64 data tables for 15 moderators based on ENDF/B-VI Release 3 evaluations. There are some substantial enhancements from previous MCNP thermal data tables that warrant the data on SAB2002 being the new default for MCNP.

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